

Analysis output: all-atom contacts and geometry for pembrolizumab_abb2_1FH.pdb



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Summary statistics

All-Atom Contacts	Clashscore, all atoms:	0.57	99 th percentile * (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	6	3.08%	Goal: <0.3%
	Favored rotamers	181	92.82%	Goal: >98%
	Ramachandran outliers	1	0.44%	Goal: <0.05%
	Ramachandran favored	221	97.36%	Goal: >98%
	Rama distribution Z-score	-1.59 ± 0.53		Goal: abs(Z score) < 2
	MolProbity score ^	1.19		99 th percentile * (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	0 / 1840	0.00%	Goal: 0%
	Bad angles:	9 / 2497	0.36%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	2 / 10	20.00%	Expected: ≤1 per chain, or ≤5%
Low-resolution Criteria	CaBLAM outliers	3	1.3%	Goal: <1.0%
	CA Geometry outliers	0	0.00%	Goal: <0.5%
Additional validations	Chiral volume outliers	0/269		
	Waters with clashes	0/0	0.00%	See UnDowser table for details

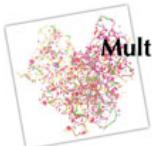
In the two column results, the left column gives the raw count, right column gives the percentage.

* 100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

^ MolProbity score combines the clashscore, rotamer, and Ramachandran evaluations into a single score, normalized to be on the same scale as X-ray resolution.

Key to table colors and cutoffs here: [?](#)

Multi-criterion visualizations



Multi-criterion kinemage

[View in KiNG](#) | [View in NGL](#) | [Download \(961 Kb\)](#)



Multi-criterion chart

[View \(279 Kb\)](#)



UnDowser

[View \(2.8 Kb\)](#)

Single-criterion visualizations

- Clash list (256 bytes): [View](#)
- Ramachandran plot kinemage (419 Kb): [View in KiNG](#) | [View in NGL](#) | [Download](#)
- Ramachandran plot PDF (1.7 Mb): [View](#)
- Ramachandran distribution Z-score analysis (12 Kb): [View](#)
- Chiral volume report (788 bytes): [View](#)
- Cβ deviation scatter plot (18 Kb): [View in KiNG](#) | [View in NGL](#) | [Download](#)

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